

MLS000736649
6640-53-5 | DTXSID10287108

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.28e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.80e-01

Confidence level: 3.38e-01

Nearest Neighbors from the Training Set

Image not found

Methylcyclopentane

Measured: 9.75e-11

Predicted: 80.1

Image not found

Hydroprene

Measured: 3.39e-09

Predicted: 8.80e-04

Image not found

2,3-Benzofluorene

Measured: 1.35e-04

Predicted: 2.22e-07

Image not found

Fluorene

Measured: 7.50e-07

Predicted: 9.71e-04

Image not found

Triphenylene

Measured: 2.08e-05

Predicted: 1.87e-08